

3-Methylhexane
589-34-4 | DTXSID3044334

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 300

Global applicability domain: Inside

Local applicability domain index: 6.95e-01

Confidence level: 7.46e-01

Nearest Neighbors from the Training Set

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Methylcyclohexane

Measured: 186

Predicted: 233

[Image not found](#)

Dibenzofuran

Measured: 1510

Predicted: 14.2

[Image not found](#)

1-Methoxynaphthalene

Measured: 162

Predicted: 11.2

[Image not found](#)

Dicyclopentadiene

Measured: 219

Predicted: 228

[Image not found](#)

Carbazole

Measured: 170

Predicted: 10.1